

# A Gamut of Hohenberg-Kohn Properties

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The Hohenberg-Kohn theorem is a cornerstone of electronic density functional theory, yet its traditional proof requires the *assumption* that ground state wavefunctions never vanish on sets of nonzero Lebesgue measure. Available unique continuation results cannot bridge the gap, uniformly in particle number, except for locally bounded potentials. Based on a simple physical intuition, the issue is approached here from a density-centric perspective. We prove some “HK properties” for interaction and external potentials in specific classes of unbounded potentials. For a class containing potentials with weak- $L^3$  attractive and locally weak- $L^3$  repulsive parts, if there is any single-particle potential in that class having a given density as ground-density, then it is unique up to a constant over the region where the density does not vanish. For a class of potentials including Kato class, the potential is unique up to a constant, if the density is everywhere nonzero. Along the way, an elementary and self-contained proof is given for molecular potentials of the classic (strong) HK property, uniqueness of the external potential up to a global constant.

## 1. INTRODUCTION

The Hohenberg-Kohn (HK) Theorem<sup>1</sup> (sometimes-designated “first”) is one of the most basic principles of density functional theory (DFT). It states that, for a system of identical interacting particles, a given particle density  $\rho(x)$  is realized as a ground state density for at most at most a single one-body potential, modulo constants. This is considered a cornerstone of DFT since, as Martin<sup>2</sup> puts it, “Therefore all properties of the system are completely determined given only the ground-density  $n_0(\mathbf{r})$ .” There is, however, a frequently-glossed-over gap in the beguilingly simple near-proof of the theorem: it is implicitly assumed that an eigenstate wavefunction cannot vanish on a set of nonzero Lebesgue measure. To show that such is indeed the case is a problem of “unique continuation”. Unfortunately, available unique continuation results are ill-suited to the needs of density functional theory. For DFT, one wants constraints on the potential which are independent of the number of particles in the system, but the best general results (reviewed in Section 3) degenerate in that case to requiring local boundedness of the potential.

Precisely where is the problem with the HK theorem? What Hohenberg & Kohn<sup>1</sup> fully proved is that if two one-body potentials have a common ground state *density*, then they have a common ground *state*. Using the constrained-search<sup>3</sup> idea, which developed later, this is easy to see. The external potential enters the total energy only via the integral  $\int \rho(x) v(x) dx$ . So, if  $\rho$  is a ground-density, then, among all states with density  $\rho$ , every one which minimizes the intrinsic (kinetic plus interaction — see Section 2) energy must be a ground state. So far, so good. To finish the proof, therefore, it needs to be shown that potentials which are not equal modulo constants cannot have a common ground state. Hohenberg and Kohn simply assert that it is so. Following textbook treatments<sup>4-6</sup>, we flesh out the presumably intended argument: With  $H_0$  denoting the sum of kinetic and interparticle interaction energy and  $V$  and  $V'$  being the  $N$ -body potentials derived from some one-body potentials, suppose that  $\psi$  is a ground state for both, so that  $(H_0 + V)\psi = 0$  and  $(H_0 + V')\psi = 0$ , in distribution sense. (Without essential loss, we take the total energies to be zero by shifting the potentials.) Subtraction yields  $(V - V')\psi = 0$ , almost everywhere. We would like to conclude from this that  $V = V'$  almost everywhere. That, however, seems to require a warrant that  $\{\psi = 0\}$  has zero Lebesgue measure, something which is not at all evident. One might hope that the special form of potentials  $V$  of interest — sums of one-body and two-body terms — would help. In the density-centered approach taken here, that fact will be exploitable.

We will work from a physically appealing intuition, expressed in terms of density and described in the next paragraph, about why the HK theorem could be expected. The mathematical goals, reached in Section 4, are proofs of *HK properties* for certain classes of potentials. Some definitions are in order:

**Definition 1.1.** For a class  $\mathcal{V}$  of one-body potentials,  $\mathcal{V}(v_{\text{int}}, \rho)$  denotes the set of potentials in  $\mathcal{V}$  for which  $\rho$  is a ground-density with interaction potential  $v_{\text{int}}$ . For a set  $A$  of functions,  $\Delta A = \{f - g : f, g \in A\}$ . (This is all just word-saving notation.)

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$\mathcal{V}$  has the *strong HK property* [relative to  $v_{\text{int}}$ ] if for every  $\rho$ ,  $\Delta\mathcal{V}(v_{\text{int}}, \rho)$  contains only constants. It has the *weak HK property* if for every  $\rho$ , elements of  $\Delta\mathcal{V}(v_{\text{int}}, \rho)$ , restricted to  $\{\rho > 0\}$  are constants. It has the *local HK property* if for every lower semicontinuous  $\rho$ , elements of  $\Delta\mathcal{V}(v_{\text{int}}, \rho)$  are constant over each connected component of  $\{\rho > 0\}$ .

Even the largest class of potentials we deal with will guarantee lower semicontinuous ground-densities, so the local HK property is not really specially restricted in scope. (But, see around 54 for a discussion of the annoying zero-measure issues.) With  $v_{\text{int}}$  in the same class, we show the local HK, weak HK and strong HK property for  $\mathcal{V}_{\text{lg}}$ ,  $\mathcal{V}_{\text{md}}$  and  $\mathcal{V}_{\text{sm}}$ , respectively. These classes are precisely defined in (6), but are a somewhat complicated. The reader may find it helpful to substitute these cut-down versions:

$$\begin{aligned}\mathcal{V}_{\text{lg}}^0 &:= \{v : v^+ \in L_{\text{wk,loc}}^2(\mathbb{R}^3), v^- \in L_{\text{wk}}^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)\} \subset \mathcal{V}_{\text{lg}}, \\ \mathcal{V}_{\text{md}}^0 &:= \{v : v^+ \in L_{\text{wk,loc}}^3(\mathbb{R}^3), v^- \in L_{\text{wk}}^3(\mathbb{R}^3)\} \subset \mathcal{V}_{\text{md}}, \\ \mathcal{V}_{\text{sm}}^0 &:= \{v \in \mathcal{V}_{\text{md}}^0 : v \text{ locally bounded away from a finite number of points}\} \subset \mathcal{V}_{\text{sm}},\end{aligned}\tag{1}$$

where  $v^+ = \max(0, v)$  and  $v^- = -\min(0, v)$  are the positive and negative parts of  $v$ . (Weak  $L^p$  spaces are also explained in Section 2). The local HK property of  $\mathcal{V}_{\text{lg}}$  may not be very useful as it stands. But, if  $\rho$  is everywhere nonzero, it is enough to secure uniqueness of the potential up to a simple constant. Insofar as this seem to be the normal situation for interacting many-body systems (and note that  $\rho > 0$  everywhere is compatible with the wavefunction vanishing on a set of nonzero measure), the theorem may be more powerful than it looks at first. As for the weak HK property of  $\mathcal{V}_{\text{md}}$ , if  $v_{\text{int}}$  is further restricted to  $\mathcal{V}_{\text{sm}}$ , then even something can be said about the behavior of the external potential where the density vanishes: roughly speaking, the singularities of the potential must be essentially dense in  $\{\rho = 0\}$  (see Sec. 4 for precise statements).

Now, to sketch the basic idea of the current approach, if  $\rho_0$  is a ground-density for  $v$ , with corresponding wavefunction  $\psi_0$ , then it is stable, in the sense that any deformation will raise the total energy, to second order. Changing the potential to  $v'$ , differing from  $v$  by more than a constant, *ought* to destabilize  $\rho_0$  — some small deformation will lower the total energy. If that is demonstrated, then  $\rho_0$  cannot be a ground-density for  $v'$ . One way to get useful deformations is to conceive of  $\rho_0$  as the density of a classical compressible fluid, with a smooth velocity field  $\mathbf{u}$  imposed, and let it run for a short time. With  $\rho_s$  the density at “time”  $s$ , and  $\psi_s$  the corresponding wavefunction, the total energy  $E(s) = \langle \psi_s | H_0 | \psi_s \rangle + \int v \rho_s dx$  must satisfy  $dE(0)/ds = 0$ . Supposing that  $\rho_0$  actually is a ground-state density for  $v'$  as well, subtraction yields  $\frac{d}{ds} E'(s)|_{s=0} = \frac{d}{ds} [E'(s) - E(s)]|_{s=0} = \int (v' - v) \operatorname{div}(\mathbf{u} \rho_s) dx$ . (Notice the strong parallel here with the argument of Hohenberg & Kohn.) At this point, the problem is reduced to merely finding  $\mathbf{u}$  that renders that final integral nonzero (if the sign is wrong, run time the other way). A loose requirement like that should be satisfied for a  $\mathbf{u}$  which is smooth and compactly supported. With potentials and  $\nabla \rho_0$  locally square integrable, the integral is well-defined and the program appears feasible. But,  $\nabla \rho_0$  is not necessarily square integrable. If the first major idea of this paper is to generate a smoothly varying family of densities using a velocity field in a hydrodynamic analogy, and lift that into ( $\mathcal{N}$ -particle) configuration space in a canonical way to obtain a corresponding family of wavefunctions, then the second is that the configuration space velocity field must be modified because the canonical lift does not have bounded support. That is the way we will cope with possible discontinuity and unboundedness of the density.

Here is brief outline of the body of the paper. Section 2 provides some relevant background on DFT and the mathematical approach to quantum mechanics. It also gives the precise definitions (6) of the classes of potentials —  $\mathcal{V}_{\text{lg}}$ ,  $\mathcal{V}_{\text{md}}$ , and  $\mathcal{V}_{\text{sm}}$  — that we use and unpacks their meaning a little. Unique continuation properties (UCPs) are considered in Section 3. Roughly, a UCP justifies the conclusion that a function in a certain class vanishes identically if it is known merely to vanish in some limited sense — on an open set (weak UCP), a set of nonzero measure (measure UCP) or to infinite order at a point (strong UCP). Section 3A explains the types, and reviews known UCPs which are relevant. That a strong UCP implies a measure UCP under assumptions on the potential is discussed in Section 3B, and a result of that type adapted to sums of one- and two-body potentials is proven. The heart of the paper is Section 4, where the HK properties are finally tackled. In Section 4A, we prove, in Thm. 4.1, the strong HK property for classes of potentials each pair of which are analytic on a full measure connected open set. Some such classes include molecular potentials. This result is interesting because it is elementary and self-contained. It also shows that a strong HK property can result for reasons having little to do with the behavior of densities or wavefunctions, but merely because the considered class of potentials is very restricted. Section 4B is the heart of the paper; the main theorems are proven there. After the basic ideas of the construction are layed out in Section 4B1, three main theorems are proven in Section 4B2. Thms. 4.2, 4.3 and 4.4 assert the local, weak and strong HK property, respectively, for  $\mathcal{V}_{\text{lg}}$  (with  $v_{\text{int}} \in \mathcal{V}_{\text{lg}}$ ),  $\mathcal{V}_{\text{md}}$  (with  $v_{\text{int}} \in \mathcal{V}_{\text{md}}$ ) and  $\mathcal{V}_{\text{sm}}$  (with  $v_{\text{int}} \in \mathcal{V}_{\text{sm}}$ ), respectively. Section 5 attempts an assessment of the results in the context of a critical discussion of the rôle of the Hohenberg-Kohn theorem in DFT. The reader uninterested in the technical details may be satisfied to glance through the notation in Section 2, read the discussion in Section 4B1 and the theorem statements in Section 4B2, and then turn to Section 5.

## 2. BACKGROUND: FUNCTIONAL ANALYSIS AND DENSITY FUNCTIONAL THEORY

In this section, we give some background and set up notations. Readers desiring more details on the mathematical approach to quantum mechanics are advised to consult<sup>7–11</sup>. Additional sources on sesquilinear forms are<sup>12–14</sup>. Sobolev spaces are discussed in<sup>15–17</sup>, as well as nearly every modern graduate text on partial differential equations. For textbook treatments of DFT, with applications, see<sup>2,4–6,18,19</sup>.

We deal with a system of an arbitrary but fixed number,  $\mathcal{N}$ , of identical non-relativistic particles in three dimensions. Everything we do will be valid for fermions or bosons of any spin. The Hilbert space of pure states,  $\mathcal{H}_{\mathcal{N}}$ , comprises wavefunctions of the appropriate symmetry, with inner product

$$\langle \psi | \phi \rangle = \sum_{\underline{\sigma}} \int \bar{\psi}(\underline{\sigma}; \underline{x}) \phi(\underline{\sigma}; \underline{x}) dx_1 \cdots dx_{\mathcal{N}}, \quad (2)$$

the sum being over all spin assignments  $\underline{\sigma} := (\sigma_1, \sigma_2, \dots, \sigma_{\mathcal{N}})$  to the  $\mathcal{N}$  particles. The Hamiltonian of this system is built from one-body and two-body pieces:

$$H = T + \Gamma v_{\text{int}} + \Gamma v = H_0 + \Gamma v, \quad (3)$$

where  $T$  denotes the kinetic energy, realized as the self-adjoint representation of  $-\nabla^2$  (depending on context, this may be the 3 or  $3\mathcal{N}$ -dimensional Laplacian),

$$\Gamma v_{\text{int}} := (x_1, \dots, x_{\mathcal{N}}) \mapsto \sum_{1 \leq i < j \leq \mathcal{N}} v_{\text{int}}(x_i - x_j) \quad (4)$$

is the interaction amongst the particles, and

$$\Gamma v := (x_1, \dots, x_{\mathcal{N}}) \mapsto \sum_{i=1}^{\mathcal{N}} v(x_i). \quad (5)$$

that with an external one-body potential.  $\Gamma$  is a generic transformation boosting one- or two-body operators into operators on the multi-particle Hilbert space in an obvious way. Generally, the interaction potential is regarded as fixed, though we do not commit to any particular choice, thus it is often convenient to combine the kinetic and interaction energy into  $H_0$  as in (3). Hamiltonians will be regarded not only as operators, but also as (quadratic, or sesquilinear) forms; the form version of operator  $A$  is denoted  $\llbracket A \rrbracket$ ; we use the Dirac notation “ $\langle \phi | A | \psi \rangle$ ” for the evaluation of  $\llbracket A \rrbracket$  on the pair  $(\phi, \psi)$ . For the physically-minded reader, we remark that an observable/operator can appear as an operation transforming state vectors into other state vectors [i.e.,  $\psi \mapsto A\psi$ ]; this is the operator version. Alternatively, it is something to take expectation values of [i.e.,  $\psi \mapsto \langle \psi | A | \psi \rangle$ ]; this is the form version. If  $A$  is unbounded, then it has a larger domain in the second guise. That renders the use of quadratic forms mathematically advantageous, but it is worth remarking that DFT deals principally in expectation values and that even the particle density can be regarded as a function-valued quadratic form. Thus, the use of quadratic forms in DFT is very natural.

The primary classes of potentials which we shall use are

$$\begin{aligned} \mathcal{V}_{\text{lg}} &:= \{v : v^+ \in K_3^{\text{loc}}, v^- \in K_3\}, \\ \mathcal{V}_{\text{md}} &:= \{v \in \mathcal{V}_{\text{lg}} : v \in M_{\text{loc}}(W^{1,2}(\Omega) \rightarrow W^{0,2}(\Omega)) \text{ for some connected open } \Omega \text{ dense in } \mathbb{R}^3\}, \\ \mathcal{V}_{\text{sm}} &:= \{v \in \mathcal{V}_{\text{md}} : v \in L_{\text{loc}}^{\infty}(\Omega) \text{ for some open } \Omega \text{ dense in } \mathbb{R}^3\}, \end{aligned} \quad (6)$$

In order, the subscripts here stand for “large”, “medium”, “small”. An even smaller class (“molecular”) of some interest is

$$\mathcal{V}_{\text{mol}} := \left\{ v(x) = \sum_{i=0}^n \frac{Z_i}{|x - x_i|} : \text{for some } n < \infty, Z_i \in \mathbb{R} \right\}. \quad (7)$$

$\mathcal{V}_{\text{mol}}$  is not directly involved in our results, although in Section 4 A, we will consider classes between  $\mathcal{V}_{\text{mol}}$  and  $\mathcal{V}_{\text{sm}}$ . The definitions of  $\mathcal{V}_{\text{lg}}$  and  $\mathcal{V}_{\text{md}}$  require clarification.  $K_n^{\text{loc}}$  is the local Kato class in  $n$  dimensions, defined (for  $n \geq 3$ ) by

$$V \in K_n^{\text{loc}} \quad \equiv \quad \forall R < \infty, \lim_{\alpha \downarrow 0} \left[ \sup_{|x| \leq R} \int_{|x-y| \leq \alpha} \frac{|V(y)|}{|x-y|^{n-2}} d^m y \right] = 0. \quad (8)$$

$K_n$  is defined similarly, but with no restriction on  $|x|$ . Note that

$$L^2(\mathbb{R}^3) \subseteq K_3, \quad (9)$$

as follows by Cauchy-Schwarz inequality. The reason for basing  $\mathcal{V}_{\text{lg}}$  on the Kato class is the following. If  $v$  is in  $K_3$  or  $K_3^{\text{loc}}$ , then  $\Gamma v$  is in  $K_{3\mathcal{N}}$  or  $K_{3\mathcal{N}}^{\text{loc}}$ , respectively [Aizenman & Simon<sup>20</sup>, Thm. 1.4(ii)]. Therefore, with  $v, v_{\text{int}} \in \mathcal{V}_{\text{lg}}$ , if  $\psi$  is an eigenfunction of  $T + \Gamma v + \Gamma v_{\text{int}}$ , then  $\psi$  is continuous [*loc. cit.*, Thm. 1.5]. See also Ref. 21 for these points. Continuity of  $\psi$  implies lower semicontinuity of the density  $\text{dens } \psi$  (defined in (16) below). This fact is of utmost importance for the approach taken in this paper. Now, in any dimension  $n$ , with  $V_+ \in K_{n,+}$ ,  $\llbracket T + V_+ \rrbracket$  is a positive, densely defined closed quadratic form, and  $C_c^\infty(\mathbb{R}^n)$  is a form core [Lemma VI.4.6c of Kato<sup>14</sup>]. Also,  $v \in K_3$  is form bounded with respect to  $T$ , with bound less than 1 [Lemma VI.4.8a, *loc. cit.*]. This means that

$$|\langle \psi | v | \psi \rangle| \leq a \langle \psi | T | \psi \rangle + b \|\psi\|^2, \quad \text{with } a < 1. \quad (10)$$

Therefore,  $\llbracket T + \Gamma v + \Gamma v_{\text{int}} \rrbracket$  is also a densely defined, semibounded, closed quadratic form with form core  $C_c^\infty(\mathbb{R}^{3\mathcal{N}})$ .

Turning to  $\mathcal{V}_{\text{md}}$ ,  $W^{k,2}(\Omega)$  is the Sobolev spaces of functions with square integrable distributional derivatives up to order  $k$ . They are Hilbert spaces; the inner product of  $W^{1,2}$  is

$$\langle f | g \rangle_{W^{k,2}(\Omega)} = \int_{\Omega} \bar{f} g + \nabla \bar{f} \cdot \nabla g \, dx, \quad (11)$$

and ‘ $W^{0,2}$ ’ is just another name for  $L^2$ .  $M(W^{k,p}(\Omega) \rightarrow W^{l,q}(\Omega))$  is a space of *Sobolev multipliers*<sup>22,23</sup> — functions which, acting via pointwise multiplication, realize bounded operators from  $W^{k,p}$  to  $W^{l,q}$ . The corresponding space of local multipliers comprises functions  $f$  such that  $f\eta \in M(W^{k,p}(\Omega) \rightarrow W^{l,q}(\Omega))$  for every  $\eta \in C_c^\infty(\Omega)$ . A complete characterization of the spaces of Sobolev multipliers is unfortunately not simple, but can be given in terms of Bessel capacities [Sec. 2.3 of Ref. 23]. We note that

$$L_{\text{wk}}^3(\Omega) \subseteq M(W^{1,2}(\Omega) \rightarrow W^{0,2}(\Omega)), \quad (12)$$

as follows from Cor. 2.3.5 of Ref. 23.  $L_{\text{wk}}^3$  is the space of weak  $L^3$  functions<sup>24</sup>. With  $\mu_f(t) = |\{x : |f(x)| > t\}|$  ( $|\cdot|$  denotes Lebesgue measure), weak  $L^p$  quasinorms are defined by

$$\|f\|_{p,\text{wk}}^p := \sup_t t^{p-1} \mu_f(t), \quad (13)$$

and a function is in  $L_{\text{wk}}^p$  if its weak- $L^p$  quasinorm is finite. By comparison, the ordinary  $L^p$  norm can be expressed as

$$\|f\|_p^p = \int_0^\infty \mu_f(t) p t^p \, dt. \quad (14)$$

To give some idea of what is included in  $L_{\text{wk}}^3(\mathbb{R}^3)$ : a simple check shows that the Coulomb potential of a point charge is so. Since  $\|f+g\|_{3,\text{wk}} \leq 2^{1/3}(\|f\|_{3,\text{wk}} + \|g\|_{3,\text{wk}})$  (this is what makes it a *quasinorm*), an everywhere dense countable sum of such Coulomb singularities is also weak- $L^3$ , if the sum of the absolute charges is finite. One hastens to add that the inclusion in  $\mathcal{V}_{\text{md}}$  (and even  $\mathcal{V}_{\text{sm}}$ ) of Coulomb potentials for isolated point charges is clear even apart from these considerations, since the singularities can be put in the exceptional set  $\mathbb{R}^3 \setminus \Omega$ . It is also easy to see that the ordinary (as opposed to weak) Lebesgue space  $L^3(\mathbb{R}^3)$  is contained in  $M(W^{1,2}(\Omega) \rightarrow W^{0,2}(\Omega))$  using just Hölder and Sobolev inequalities:

$$\|Vf\|_2 \leq \|V\|_3 \|f\|_6 \leq \|V\|_3 \|f\|_{W^{1,2}}. \quad (15)$$

Associated to the state vector  $\psi \in \mathcal{H}_{\mathcal{N}}$  is the particle density

$$\text{dens } \psi(x_1) = \mathcal{N} \sum_{\underline{g}} \int |\psi(\underline{g}; x_1, x_2, \dots, x_N)|^2 dx_2 \cdots dx_N = \mathcal{N} \int |\psi|^2 d\sigma dx_{\perp}. \quad (16)$$

The final expression indicates a compressed notation which we shall prefer. The total energy of state  $\psi$  in presence of the one-body potential  $v$  is

$$\begin{aligned} \mathcal{E}_v(\psi) &= \langle \psi | H_0 + \Gamma v | \psi \rangle = \langle \psi | H_0 | \psi \rangle + \int v(x) \text{dens } \psi(x) \, dx \\ &= \mathcal{E}_0(\psi) + \langle v, \text{dens } \psi \rangle. \end{aligned} \quad (17)$$

$\mathcal{E}_0(\psi) = \langle \psi | H_0 | \psi \rangle$  is called the *intrinsic energy* of state  $\psi$ . Both the intrinsic energy ( $\mathcal{E}_0$ ) and the particle density function (**dens**) naturally extend linearly to mixed states  $\gamma = \sum \lambda_i |\psi_i\rangle\langle\psi_i|$  as **dens**  $\gamma = \sum \lambda_i$  **dens**  $\psi_i$ , and  $\mathcal{E}_0(\gamma) = \sum \lambda_i \mathcal{E}_0(\psi_i)$ . The intrinsic energy of a *density*  $\rho$  is

$$F(\rho) := \inf\{\mathcal{E}_0[\gamma] \mid \text{dens } \gamma = \rho\}. \quad (18)$$

The minimization is carried out over mixed states with the prescribed density. If  $v_{\text{int}} \in \mathcal{V}_{\text{lg}}$ ,  $F(\rho)$  is finite if and only if  $\sqrt{\rho} \in W^{1,2}(\mathbb{R}^3)$ . Using the Cauchy-Schwarz inequality,  $|\nabla \rho(x_1)|^2 \leq 4\mathcal{N}\rho(x_1)\mathcal{N} \int |\nabla_1 \psi|^2 d\sigma dx_\perp$ , and “only if” follows<sup>25,26</sup> immediately from this and form boundedness of the negative part of  $v_{\text{int}}$ . [See §VI.4.3 of Ref.<sup>14</sup> for interactions in Kato class.] If this condition fails, then  $\rho$  cannot be a ground-state density of a  $\mathcal{V}_{\text{lg}}$  potential. Thus, we are only interested in densities with  $F < \infty$ . We do not actually need the “if” direction, but we note that the weak constraints on  $v_{\text{int}}^+$  cannot cause any density to have infinite intrinsic energy because it can always be realized by a mixed state, no component of which has any two particles far separated.

### 3. UNIQUE CONTINUATION

This section is concerned with unique continuation properties (UCPs) which are relevant to the Hohenberg-Kohn problem and relations between them. Roughly, a UCP says that, in some context, a function vanishing on a “small” set vanishes everywhere. The obvious types of “vanishing on a small set” are vanishing on some open set (weak UCP) or on a set of nonzero measure (here designated measure UCP). It is this second sort which would seem immediately relevant to our problem. Technically very important is a third mode — vanishing to infinite order at a point (strong UCP). Section 3A reviews results we will need, and Section 3B gives a tailor-made extension of known results on the reduction of measure UCP to strong UCP. The results of this section enter the proofs of Section 4 at just a few discrete points, hence it can probably be skipped until called for.

#### A. UCP varieties and results

The usual context of a *unique continuation property* (UCP) is a differential inequality such as

$$|\nabla^2 u| \leq |Vu|, \quad (19)$$

on some connected open set  $\Omega \subseteq \mathbb{R}^n$ . A UCP asserts that if  $u$  satisfies (19) for some  $V$  in a class of functions  $\mathcal{V}$  and has a property  $P$  of “vanishing in a weak sense”, then it is identically zero on  $\Omega$  (almost everywhere). There seem to be three basic vanishing properties in this context. We speak of a *weak* UCP if  $P(u) \equiv$  “ $u$  vanishes almost everywhere on a nonempty open set”, and of a *strong* UCP if  $P(u) \equiv$  “ $u$  vanishes to infinite order at some point in  $\Omega$ ”. The function  $u$  is said to vanish to infinite order at  $y$  if

$$\forall N \in \mathbb{N}, \quad \int_{B(y,r)} |u|^2 dx = \mathcal{O}(r^N) \quad \text{as } r \rightarrow 0. \quad (20)$$

The adjectives ‘weak’ and ‘strong’ in this context seem to be fairly standardized. A third local vanishing property, and the one which most immediately concerns us is  $P(u) \equiv$  “ $u$  vanishes on a set of nonzero Lebesgue measure”. We will call a UCP with this local vanishing property a *measure* UCP.

More generally, a UCP concerns a class  $\mathcal{F}$  of functions defined by a differential inequality such as (19) or a differential equation, and dependent on an auxiliary class  $\mathcal{V}$ . Clearly, for any class  $\mathcal{F}$ , both the strong UCP and the measure UCP imply the weak UCP. It is not immediately clear how strong and measure UCPs compare, but it is an important question to which we return shortly.

The best strong UCP for (potentials in)  $L^p$  spaces is

**Theorem 3.1** (Jerison and Kenig<sup>27</sup>). *Suppose, with  $n \geq 3$ ,  $q = 2n/(n+2)$ , and  $\Omega$  a connected open subset of  $\mathbb{R}^n$ , that  $u \in W_{\text{loc}}^{2,q}(\Omega)$  satisfies (19) for  $V \in L_{\text{loc}}^{n/2}(\Omega)$ . Then, if  $u$  vanishes to infinite order at any point, it is identically zero.*

For application to density functional theory,  $n = 3\mathcal{N}$  and we want constraints on the one-body and interaction potentials which are uniform in the number of particles  $\mathcal{N}$ . In that context, the result of Jerison and Kenig is no more powerful than if  $L^{n/2}$  were replaced by  $L^\infty$ . The strong UCP for the latter class of potentials was already proved by Müller<sup>28</sup>.

For that reason, a weak UCP of Schechter and Simon will be useful. It is tailor-made to our context of one- and two-body potentials.



**Theorem 3.2** (Schechter & Simon Thm. 2.1<sup>29</sup>). *Suppose  $V$  satisfies*

$$\|Vu\|_{L^2(B)}^2 \leq C(\|u\|_{L^2(B)}^2 + \|\nabla u\|_{L^2(B)}^2) \quad (21)$$

*for some constant  $C$ , ball  $B$  of radius less than 1, and all  $u \in C_c^\infty(B)$ . Then, if (19) holds, and  $u$  vanishes on any ball inside  $B$ ,  $u \equiv 0$  on  $B$ .*

Note that the expression on the right-hand side of the condition (21) is the  $W^{1,2}(B)$  norm squared. Thus, we can rephrase the consequences of this theorem as giving a weak UCP with  $\mathcal{V}$  being the space  $M_{\text{loc}}(W^{1,2}(\Omega) \rightarrow W^{0,2}(\Omega))$  of local Sobolev multipliers.  $v$  is in this space if, for any  $\eta \in C_c^\infty(\Omega)$ ,  $\eta v$  is in the Sobolev multiplier space<sup>22,23</sup>  $M(W^{1,2}(\Omega) \rightarrow W^{0,2}(\Omega))$ . From Cor. 2.3.5 of<sup>23</sup> or Prop. 1 of §1.3.4 of<sup>22</sup>, it follows that  $L_{\text{wk,loc}}^3(\Omega) \subseteq M_{\text{loc}}(W^{1,2}(\Omega) \rightarrow W^{0,2}(\Omega))$ .

## B. vanishing on set of nonzero measure implies a zero of infinite order

For  $L^{n/2}$  potentials in the  $n$ -dimensional Schrödinger equation, a measure UCP is implied by the Jerison & Kenig strong UCP. This was shown by de Figueiredo & Gossez<sup>30</sup>. Regbaoui<sup>31</sup> has extended the reduction to differential inequalities with a first-order derivative term. In contrast to the reduction of a weak UCP to either a strong UCP or measure UCP, it is not trivial or automatic. The reduction immediately yields a strong HK property which will be stated as Thm. 4.4, but it imposes rather strong restrictions on the potentials.

In this section, we deviate from our standing assumption of three-dimensionality, instead working in general dimension  $d$ , and adapt the proof of<sup>30</sup> to the specific context of one- and two-body potentials. Prop. 3.1 below implies that if  $\rho$  vanishes on a set  $A$  of nonzero measure, then  $\psi$  vanishes to infinite order at almost every point of  $A^\mathcal{N}$ . Unfortunately, an appropriate strong UCP which takes full advantage of Prop. 3.1 is not available. In terms of what we will be able to do with it here, it does not improve on the result of<sup>30</sup>, which already licenses the replacement of “vanishes to infinite order at some point” in the Jerison & Kenig UCP by “vanishes on a set of nonzero measure”. But, it does at least make the paper more self-contained.

**Proposition 3.1.** *With  $D \equiv Nd$ ,  $v$  and  $v_{\text{int}}$  in  $L_{\text{loc}}^{d/2}(\mathbb{R}^d)$  and  $V = \Gamma v + \Gamma v_{\text{int}}$ , suppose  $\psi \in H_{\text{loc}}^1(\mathbb{R}^D)$  is a weak solution of the Schrödinger equation  $(-\nabla^2 + V)\psi = 0$ . Then, if  $\psi$  vanishes on a set  $Z$  of nonzero measure, it vanishes to infinite order at almost every point of  $Z$ .*

We begin with

**Lemma 3.1.** *Since each spin component of  $\psi$  satisfies the Schrödinger equation, it is only necessary to prove the spinless case. The weak formulation is then*

$$\int \nabla \psi \cdot \nabla \bar{\eta} d^D x + \int V \psi \bar{\eta} d^D x = 0, \quad \forall \eta \in C_c^\infty(\mathbb{R}^D). \quad (22)$$

With  $B(x; r)$  denoting the open ball of radius  $r$  about an arbitrary point  $x \in \mathbb{R}^D$  (later we drop the ‘ $x$ ’), for  $r$  small enough,

$$\int_{B(x;r)} |\nabla \psi|^2 d^D x \leq \frac{c(x)}{r^2} \int_{B(x;2r)} |\psi|^2 d^D x. \quad (23)$$

*Proof.* Take  $h : \mathbb{R}^D \rightarrow [0, 1]$  a smooth bump function equal to 1 on  $B(x; r)$  and supported on  $B(x; 2r)$ , with  $|\nabla h| \leq 2/r$ . In (22), substitute  $h^2 \psi$  for  $\eta$  (the first integral and the right-hand side are continuous in  $\eta$  with respect to  $W^{1,2}$  norm). Then,

$$\int |h \nabla \psi|^2 = -2 \int h \nabla \psi \cdot \bar{\psi} \nabla h - \int V |h \psi|^2 \quad (24)$$

We intend to bound the terms on the right-hand side. The first term is quickly dispatched:

$$\left| 2 \int h \nabla \psi \cdot \bar{\psi} \nabla h \right| \leq 2 \|h \nabla \psi\|_2 \|\psi \nabla h\|_2 \leq \frac{1}{3} \|h \nabla \psi\|_2^2 + 3 \|\psi \nabla h\|_2^2. \quad (25)$$

For the final integral in (24), recall that  $V$  is a sum of  $n = \mathcal{N}(\mathcal{N} + 1)/2$  terms. Defining

$$\tilde{\rho}(x_1) = \int |h \psi|^2 dx_\perp, \quad (26)$$

and splitting the integration domain according to whether  $|v|$  is smaller or larger than some constant  $M$ , we bound the contribution of  $v(x_1)$  to the integral in (24) by

$$M \int_{|v| < M} \tilde{\rho} d^d x + \int_{|v| \geq M} |v| \tilde{\rho} d^d x \leq M \|h\psi\|_2^2 + \|v \cdot \chi(B(x_1, 2r)) \chi(|v| \geq M)\|_{\frac{d}{2}} \|\tilde{\rho}\|_{\frac{d}{d-2}}, \quad (27)$$

where the last term was obtained by use of the Hölder inequality (and uses the assumption  $v \in L_{\text{loc}}^{3/2}$ ), and  $M$  is yet to be chosen. For the second factor in the last term, use

$$\|\tilde{\rho}\|_{\frac{d}{d-2}} = \|\tilde{\rho}^{1/2}\|_{\frac{2d}{d-2}}^2 \leq C \|\nabla \tilde{\rho}^{1/2}\|_2^2 \leq C \|\nabla(h\psi)\|_2^2, \quad (28)$$

where the first inequality is a Sobolev inequality, and the second follows from  $|\nabla \tilde{\rho}| = |2 \operatorname{Re} \int \nabla(h\psi)(h\bar{\psi}) dx_\perp| \leq 2|\tilde{\rho}^{1/2}|(\int |\nabla(h\psi)|^2 dx_\perp)^{1/2}$  as in Thm. 1.1 of<sup>25</sup>. Turning to the other factor,  $\|v \cdot \chi(B(x_1, 2r)) \chi(|v| \geq M)\|_{d/2}$ , choose  $M$  large enough that this is less than  $1/(6nC)$ , and so are the  $n-1$  similar factors arising from the other terms of  $V$ .  $M$  will, in general, depend on  $x$ . Having thusly chosen  $M$ , we obtain

$$\left| \int V |h\psi|^2 \right| \leq nM \|h\psi\|_2^2 + \frac{1}{6} \|\nabla(h\psi)\|_2^2. \quad (29)$$

Putting the bounds (25) and (29) together produces

$$\frac{1}{3} \|h\nabla\psi\|_2^2 \leq \frac{10}{3} \|\psi\nabla h\|_2^2 + nM \|h\psi\|_2^2. \quad (30)$$

With a bit of rearrangement,

$$\int_{B(x;r)} |\nabla\psi|^2 d^D x \leq \int h^2 |\nabla\psi|^2 d^D x \leq \left( nM + \frac{40}{r^2} \right) \int_{B(x;2r)} |\psi|^2 d^D x. \quad (31)$$

□

*Proof of Prop. 3.1.* Recall that  $Z$  denotes the set where  $\psi = 0$ , assumed of nonzero Lebesgue measure. Almost every point  $x \in Z$  is a point of Lebesgue density, which means that

$$\lim_{r \rightarrow 0} \frac{|Z \cap B(x;r)|}{|B(x;r)|} = 1. \quad (32)$$

It is convenient to express this in the form

$$|Z^c \cap B(x;r)| \leq [rK(r)]^D \quad (33)$$

for some monotonic function  $K : \mathbb{R}_+ \rightarrow \mathbb{R}_+$  with  $K(0) = 0$ . Then, by Hölder's inequality,

$$\int_{B(x;r)} |\psi|^2 = \int_{B(x;r) \cap Z^c} |\psi|^2 \leq \left( \int_{B(x;r) \cap Z^c} |\psi|^{\frac{2D}{D-2}} \right)^{\frac{D-2}{D}} |B(x;r) \cap Z^c|^{\frac{2}{D}} \quad (34)$$

An extension argument of the sort standardly used to produce a continuous injection of  $H^m(\Omega) \rightarrow H^m(\mathbb{R}^n)$  for bounded  $\Omega$ , followed by a Sobolev inequality, implies that the integral here is bounded as

$$\left( \int_{B(x;r) \cap Z^c} |\psi|^{\frac{2D}{D-2}} \right)^{\frac{D-2}{D}} \leq c \left( \int_{B(x;r)} |\nabla\psi|^2 + \frac{1}{r^2} \int_{B(x;r)} |\psi|^2 \right). \quad (35)$$

$$\begin{aligned} \int_{B(x;r)} |\psi|^2 &\leq cK(r)^2 \left( r^2 \int_{B(x;r)} |\nabla\psi|^2 + \int_{B(x;r)} |\psi|^2 \right) \\ &\leq cK(r)^2 \int_{B(x;2r)} |\psi|^2 \end{aligned} \quad (36)$$

It is a straight line from this inequality to the desired conclusion,  $\int_{B(x;r)} |\psi|^2 = O(r^N)$ . With the definitions

$$F(r) := \int_{B(x;r)} |\psi|^2, \quad g(2r) := cK(r)^2, \quad (37)$$

an induction starting from (36) yields  $F(2^{-n}r) \leq g(r)^n F(r)$  for  $n \in \mathbb{N}$ . Applying monotonicity of  $F$ , this strengthens to

$$F(2^{-x}r) \leq g(r)^x \frac{F(r)}{g(r)}, \quad (38)$$

for real  $x \geq 1$ , from which it immediately follows that

$$\frac{F(2^{-x}r)}{(2^{-x}r)^N} \leq [2^N g(r)]^x \frac{F(r)}{g(r)}. \quad (39)$$

With  $r$  chosen small enough that  $g(r) < 2^{-N}$ , the right-hand side tends to zero as  $x \rightarrow \infty$ , showing that  $F(r) = o(r^N)$ .  $\square$

#### 4. HK PROPERTIES

This section gets down to the actual business of proving HK properties. Section 4A proves the strong HK property for classes of potentials which are analytic off of suitably small sets. A triple of deeper results is derived in Section 4B2: local HK, weak HK and strong HK for  $\mathcal{V}_{\text{lg}}$  with  $v_{\text{int}} \in \mathcal{V}_{\text{lg}}$ ,  $\mathcal{V}_{\text{md}}$  with  $v_{\text{int}} \in \mathcal{V}_{\text{md}}$ , and  $\mathcal{V}_{\text{sm}}$  with  $v_{\text{int}} \in \mathcal{V}_{\text{sm}}$ , respectively [recall the definitions of these spaces in (6)].

##### A. an easy case: piecewise analytic potentials

With sufficiently strong restrictions on potentials, it will be automatic that  $V = V'$  either almost everywhere, or almost nowhere. We now consider an easy, but nevertheless interesting, case, namely that of potentials which are analytic off of a closed Lebesgue null set with connected complement. The key is the following simple proposition.

**Lemma 4.1.** *Suppose  $f$  is real analytic on a connected open set  $\Omega \subset \mathbb{R}^n$ . Then,  $f$  is equal to zero either everywhere or almost nowhere on  $\Omega$ .*

*Proof.* Since  $\Omega$  can be covered by a countable collection of overlapping open  $n$ -cubes, it will suffice to prove the lemma for the special case  $\Omega = (0, 1)^n$ . Writing  $P(n)$  for “the Lemma holds for  $(0, 1)^n$ ”, proceed by induction on  $n$ , using analyticity of restrictions of  $f$  to affine subspaces as follows.

$P(1)$ : This case is essentially the same as a standard result in elementary complex analysis showing that zeros are isolated. We recall the argument. Suppose  $f(y) = 0$  and a sequence  $(x_n)$  of distinct zeros of  $f$  converges to  $y$ . Then, the Taylor series expansion  $f(x) = \sum_{n \geq 1} c_n(x - y)^n$  has no constant term. But the difference quotients  $(f(x_k) - f(y))/(x_k - y)$  are all zero, so  $c_1 = 0$ . Then,  $g(x) = \sum_{n \geq 1} c_{n+1}(x - y)^n$  agrees with  $f(x)/(x - y)$  for  $x \neq y$ , is again analytic, and  $g(x_n) = 0$ . Repeating the argument over and over now shows that  $c_n = 0$  for all  $n$ .

$P(n) \Rightarrow P(n+1)$ : For  $y \in (0, 1)$ ,  $x \in (0, 1)^n$ , write  $f_y(x) = f(x, y)$  and define  $J := \{y \in (0, 1) : f_y \equiv 0\}$ . Now,  $|f^{-1}(0)| = \int_{(0,1)} |f_y^{-1}(0)| dy$ . (Recall,  $|\cdot|$  denotes Lebesgue measure.) By the induction hypothesis, if  $y \in J$ ,  $|f_y^{-1}(0)| = 1$ , otherwise  $|f_y^{-1}(0)| = 0$ , so  $|f^{-1}(0)| = |J|$ . Suppose  $|J| > 0$ . With fixed  $x \in (0, 1)^n$ ,  $f(x, y)$  is an analytic function of  $y$  vanishing on  $J$ . Then, by  $P(1)$ ,  $f(x, y) = 0$  for all  $y$ , and since  $x$  was arbitrary,  $f \equiv 0$ .  $\square$

We apply the lemma to obtain a strong HK property for subclasses of

$$\mathcal{V}_{\text{afo}} = \{v : \text{dom } v \rightarrow \mathbb{R} \text{ real analytic, with } \text{dom } v \text{ a full-measure open subset of } \mathbb{R}^3\}. \quad (40)$$

**Lemma 4.2.** *For fixed  $v_{\text{int}}$  analytic on  $\mathbb{R}^3 \setminus \{0\}$  (i.e., except at contact), if  $\rho$  is a ground-density of both  $v$  and  $v'$  in  $\mathcal{V}_{\text{afo}}$ , then over each connected component of  $\text{dom } v \cap \text{dom } v'$ , either  $v - v'$  is a constant or  $\rho$  is identically zero.*

*Proof.* Write  $\mathcal{P}$  for the set of connected components of  $\text{dom}(v' - v) = \text{dom } v' \cap \text{dom } v$ . On  $\mathbb{R}^{3N}$ ,  $W := \Gamma(v' - v)$  is again analytic on a full measure open set which has  $\mathcal{P}^N$  for its connected components. Now, suppose  $\rho$  is not a.e. zero on  $\mathcal{U} \in \mathcal{P}$ . In that case, then there must be some  $\mathcal{U} \times \tilde{\mathcal{U}} \in \mathcal{P}^N$  on which  $\psi$  is not a.e. zero. Since, following the discussion in the introduction,  $W\psi = 0$ , Lemma 4.1 implies that  $W \equiv 0$  on  $\mathcal{U} \times \tilde{\mathcal{U}}$ . With fixed  $\underline{x}_\perp \in \tilde{\mathcal{U}}$ , only  $x_1$  varies over  $\mathcal{U} \times \underline{x}_\perp \subset \mathcal{U} \times \tilde{\mathcal{U}}$ . Since  $W \equiv 0$  on this slice,  $v' - v \equiv 0$  on  $\mathcal{U}$ .  $\square$



**Theorem 4.1.** *With  $v_{int}$  analytic on  $\mathbb{R}^3 \setminus \{0\}$ , if  $\mathcal{V}$  is a subclass of  $\mathcal{V}_{af}$  with the property that  $\text{dom } v \cap \text{dom } v'$  is connected for every pair  $v, v' \in \mathcal{V}$ , then  $\mathcal{V}$  has the strong HK property.*

*Proof.* This follows immediately from Lemma 4.2 since under the given hypotheses,  $\text{dom } v \cap \text{dom } v'$  has only one connected component.  $\square$

The interest of this theorem stems largely from the fact that many classes  $\mathcal{V}$  to which it applies contain the molecular potentials (6). However, one may well feel a little unhappy with the theorem. A strong HK property is obtained for the “wrong” reasons — connected to rigidity of analytic potentials, rather than anything to do with densities or wavefunctions or the Schrödinger equation in a substantial way.

## B. HK properties for unbounded potentials

### 1. rough ideas

Suppose that  $\psi_0$ , with density  $\rho_0 = \text{dens } \psi_0$ , is a ground state of  $H_0 + \Gamma v_0$  for  $v_0 \in \mathcal{V}_{lg}$ . Imagine  $\psi_0$  in presence of  $v_0$  when, suddenly, the potential is switched to  $v' \in \mathcal{V}_{lg}$ , differing from  $v_0$  by more than a constant over some component of  $\{\rho > 0\}$ . Intuitively, one expects that it must be possible to lower *total* (not just potential) energy by shifting particle number to the regions where the potential has gone down (relative to some overall shift). Such a particle number shift may be very hard to get a grip on, mathematically, but perhaps an appropriate small, local, shift of particle number will lower the energy a little; that seems much more tractable.

To implement this idea of small, local shift of particle number, we embed  $\psi_0$  in a smoothly varying one-parameter family  $s \mapsto \psi_s : \mathbb{R} \rightarrow \mathcal{H}_{\mathcal{N}}$  of normalized wavefunctions with corresponding densities  $\rho_s = \text{dens } \psi_s$ . Since total energy is minimized at  $s = 0$ , assuming differentiability,

$$0 = \left. \frac{d}{ds} \mathcal{E}_v(\psi_s) \right|_{s=0} = \left. \frac{d}{ds} \mathcal{E}_0(\psi_s) \right|_{s=0} + \left\langle v, \frac{d\rho_s}{ds} \right\rangle \Big|_{s=0}. \quad (41)$$

Then, in presence of the second potential  $v'$ ,

$$\left. \frac{d}{ds} \mathcal{E}_{v'}(\psi_s) \right|_{s=0} = \left\langle v' - v, \frac{d\rho_s}{ds} \right\rangle \Big|_{s=0}. \quad (42)$$

If  $\psi_0$  is a ground-density also for  $v'$ , then the left-hand side of (42) is zero. If we can show that the right-hand side is *nonzero*, it will follow that  $\psi_0$  is not a ground-density for  $v'$ . To that end, we parametrize a smooth deformation family by a smooth “velocity” field  $\mathbf{u}$  such that  $d\rho_s/ds = -\text{div}(\rho_s \mathbf{u})$ . Finally, we must show that the derivatives in (41) actually exist.

We now discuss the generation of smoothly varying one-parameter families of densities and wavefunctions using velocity fields. Bokanowski and Grebert<sup>32,33</sup> used similar techniques in the context of density functional theory. Imagine a compressible fluid upon which is imposed a time-independent velocity field  $\mathbf{u}$  with continuous derivatives of all orders and vanishing outside some bounded set, i.e.,  $\mathbf{u} \in C_c^\infty(\mathbb{R}^3; \mathbb{R}^3)$ . Because the flow is steady, it generates a one-parameter group of transformations  $\Phi_s^{\mathbf{u}}$  of the density field. That is, if the density is  $\rho_0$  at time 0, then the density field is at time  $s$  is  $\rho_s = \Phi_s^{\mathbf{u}} \rho_0$ , and  $\Phi_s^{\mathbf{u}} \circ \Phi_t^{\mathbf{u}} = \Phi_{s+t}^{\mathbf{u}}$ . The infinitesimal generator of the group  $(\Phi_s^{\mathbf{u}} : s \in \mathbb{R})$  is given by the familiar continuity equation

$$\frac{d\rho_s}{ds} = -\text{div}(\rho_s \mathbf{u}) = -\mathbf{u} \cdot \nabla \rho_s - (\text{div } \mathbf{u}) \rho_s. \quad (43)$$

In our quantum mechanical context, the density derives from a wavefunction via the map  $\text{dens}$  (16), so we need to lift the action  $\Phi_s^{\mathbf{u}}$  to a one-parameter unitary group  $s \mapsto \hat{\Phi}_s^{\mathbf{u}} : \mathbb{R} \rightarrow \text{Aut}(\mathcal{H}_{\mathcal{N}})$  (unitaries) in Hilbert space satisfying  $\text{dens} \circ \hat{\Phi}_s^{\mathbf{u}} = \Phi_s^{\mathbf{u}} \circ \text{dens}$ . We take an intermediate step by applying the previous idea to a “fluid” in  $\mathcal{N}$ -particle configuration space  $\mathbb{R}^{3\mathcal{N}}$  with density  $|\psi|^2$ . Lift the velocity field  $\mathbf{u}$  into  $\mathbb{R}^{3\mathcal{N}}$  as

$$\mathbf{U} = (\mathbf{U}_1, \mathbf{U}_2, \dots, \mathbf{U}_{\mathcal{N}}) = \Gamma \mathbf{u} := (x_1, \dots, x_{\mathcal{N}}) \mapsto (\mathbf{u}(x_1), \dots, \mathbf{u}(x_{\mathcal{N}})) \quad (44)$$

Assuming we have a unitary group inducing this behavior of  $|\psi|^2$ , it gives

$$-\frac{d\rho_s}{ds}(x_1) = \mathcal{N} \int \text{div}(\mathbf{U} |\psi|^2) d\sigma dx_{\perp} = \text{div} \left( \mathbf{u}(x_1) \mathcal{N} \int |\psi|^2 d\sigma dx_{\perp} \right) = \text{div}(\mathbf{u} \rho_s)(x_1). \quad (45)$$

Only the first component of  $\mathbf{U}$  matters here; that simple fact will be important later. Finally, to make all this quantum mechanically sensible, we need to see what to do with the phase of  $\psi$ . The answer is that it is simply carried along with the flow, like a passive scalar. The generator of the unitary group corresponding to  $\mathbf{U}$  is

$$D_{\mathbf{U}} := -\mathbf{U} \cdot \nabla - \frac{1}{2} \operatorname{div} \mathbf{U}, \quad (46)$$

the second term being just a multiplicative operator. Above, we lifted  $\mathbf{u}$  to  $\mathbf{U}$  in a very simple, obvious, manner. In Thm. 4.3, it will be necessary to modify that construction. The fundamental constraint on the velocity field  $\mathbf{U}$  on configuration space is

$$\mathbf{U}_1(x_{\pi 1}, x_{\pi 2}, \dots, x_{\pi N}) = \mathbf{U}_{\pi 1}(x_1, x_2, \dots, x_N). \quad (47)$$

This is required in order that the generated unitary group preserve the symmetry or antisymmetry of the wavefunction.

Now we turn back to consider the existence of the derivatives on the right-hand side of (41).  $\mathbf{u}$  is smooth with support in some bounded ball  $B$ , and  $v$  is in  $L^2_{\operatorname{loc}}(\mathbb{R}^3)$ . Thus, with  $d\rho_s/ds$  given by (45),  $\langle v, d\rho_s/ds \rangle|_{s=0}$  makes sense as the  $L^2$  inner product  $\langle -v | \operatorname{div}(\rho_0 \mathbf{u}) \rangle$ , but only if  $\nabla \rho_0 \in L^2_{\operatorname{loc}}(\mathbb{R}^3)$ . Unfortunately, we cannot depend on that. Since  $|\nabla \rho|^2/\rho$  is square integrable (see Section 2), the obstruction is potential unboundedness of  $\rho$ . Briefly, the way we deal with this is to modify  $\mathbf{U}$  so that only part of the density is transported. The first component  $(\Gamma \mathbf{u})_1$  does not depend on positions of particles  $2-N$  and vanishes for  $x_1$  outside some bounded set. The modification we will make will cut off  $\mathbf{U}$  so that it vanishes if *any* particle is outside some bounded set. This also alleviates potential problems with the interaction energy, as we shall presently see.

The first term on the right-hand side of (41),  $d\langle \psi_s | H_0 | \psi_s \rangle / ds$ , should be made of two pieces,  $2 \operatorname{Re} \langle \psi_0 | T | D_{\mathbf{U}} \psi_0 \rangle$  and  $2 \operatorname{Re} \langle \psi_0 | \Gamma v_{\operatorname{int}} | D_{\mathbf{U}} \psi_0 \rangle$ . The kinetic energy piece is no problem, as long as  $\mathbf{U}$  and  $\operatorname{div} \mathbf{U}$  are bounded. If those conditions hold,  $D_{\mathbf{U}}$  maps  $\operatorname{dom} H_0$  into  $\operatorname{dom} [T]$ . If  $v_{\operatorname{int}}$  is in  $K_3$ , then the interaction energy term is equally easy, since such  $v_{\operatorname{int}}$  is form small with respect to  $T$ . But, if the positive part of  $v_{\operatorname{int}}$  is only restricted to  $K_3^{\operatorname{loc}}$ , the long-range part of the interaction may cause problems. To deal with that, we ask that  $|\mathbf{U}|$  and  $|\operatorname{div} \mathbf{U}|$  be bounded by  $c\chi_K$ , a multiple of the characteristic function of a compact set  $K \subset \mathbb{R}^{3N}$ . In that case, what we want to compute is essentially a matrix element of  $\chi_K \cdot \Gamma v_{\operatorname{int}} \in K_{3N}$ . Thus, with  $\mathbf{U}$  smooth and compactly supported in  $\mathbb{R}^{3N}$ , the first term on the right-hand side of (41) makes sense. Assuming we have managed to make  $d\rho/ds$  square integrable, we can now legitimately pass to

$$\left. \frac{d}{ds} \mathcal{E}_{v'}(\psi_s) \right|_{s=0} = \langle v' - v | d\rho_s/ds \rangle|_{s=0}. \quad (48)$$

## 2. proofs of main theorems

In this section, we return to a more formalized way of working. The preliminary lemmata below do not make any reference to an underlying wavefunction, and effectively show how a suitable velocity field  $\mathbf{u}$  is to be found in the case that  $v_{\operatorname{int}}$  is restricted to  $K_3$  and the particle density is in  $W^{1,2}_{\operatorname{loc}}(\mathbb{R}^3)$ . In Thm. 4.2, we use those results with a modification of the lifted velocity  $\Gamma \mathbf{u}$  to demonstrate the local HK property for  $\mathcal{V}_{\operatorname{lg}}$ , with  $v_{\operatorname{int}} \in \mathcal{V}_{\operatorname{lg}}$ . In this setting, two potentials  $v$  and  $v'$ , both with  $\rho$  as a ground-density, are shown to differ by only a constant over each connected component of  $\{\rho > 0\}$  (remember,  $\rho$  is lower semicontinuous). But those constants do not have to be the same from one component to another. In Thm. 4.3, we show that they are so if we restrict to  $\mathcal{V}_{\operatorname{md}}$ . This is the weak HK property for  $\mathcal{V}_{\operatorname{md}}$  and uses the Schechter & Simon weak UCP in a crucial way. Neither of these theorems give any information on the potentials in the region where  $\rho = 0$ . If we restrict still further, by requiring  $v_{\operatorname{int}} \in \mathcal{V}_{\operatorname{sm}}$ , then we at least can show that “singularities of  $v$  are essentially dense in  $\{\rho = 0\}$ ”: given  $c < \infty$ , for almost every point  $x$  of  $\{\rho = 0\}$ , every neighborhood of  $x$  intersects  $\{|v| > c\}$  in a set of nonzero measure. This is Thm. 4.2.

**Lemma 4.3.** *If  $\Omega$  is a connected open set, then  $\{\operatorname{div} \mathbf{J} : \mathbf{J} \in C_c^\infty(\Omega, \mathbb{R}^3)\}$  is dense in the orthogonal complement of the constants in  $L^2(\Omega)$ . (If  $\Omega$  is not bounded, this just says that  $\operatorname{ran} \operatorname{div}$  is dense in  $L^2(\Omega)$ .)*

*Proof.* Clearly,  $\operatorname{div} : C_c^\infty(\Omega, \mathbb{R}^3) \rightarrow L^2(\Omega)$  is a linear map from smooth vector fields with support contained in  $\Omega$  into square integrable functions on  $\Omega$ . Only linearity is important here, not continuity. Suppose  $f \in L^2(\Omega, \mathbb{R}^3)$  is orthogonal to the linear subspace  $\operatorname{ran} \operatorname{div}$  (range of  $\operatorname{div}$ ). Then, for  $\mathbf{J} \in C_c^\infty(\Omega, \mathbb{R}^3)$ ,

$$0 = \langle f | \operatorname{div} \mathbf{J} \rangle = \int_{\Omega} -\nabla f \cdot \mathbf{J} \, dx, \quad (49)$$

with  $\nabla f$  understood as a distribution in the final integral. Since this holds for all  $\mathbf{J} \in C_c^\infty(\Omega, \mathbb{R}^3)$  and a distribution with zero gradient is constant<sup>17,34</sup>,  $f$  is constant as a distribution, hence as an element of  $L^2(\Omega)$ . Thus, the orthogonal complement of the closure of  $\operatorname{ran} \operatorname{div}$  contains only constants, as announced.  $\square$

**Lemma 4.4.** Suppose  $\Omega$  is a connected open set, and  $\rho \in W^{1,2}(\Omega)$  is continuous with lower bound  $\rho_{\min} > 0$ . Then, for any  $w \in L^2(\Omega)$  and tolerance  $\epsilon > 0$ , there is  $\mathbf{u} \in C_c^\infty(\Omega, \mathbb{R}^3)$  such that  $\|\operatorname{div}(\rho \mathbf{u}) - w\|_{L^2(\Omega)} < \epsilon$ . In particular, the requirements are satisfied by  $\mathbf{u} = \mathbf{J}/\tilde{\rho}$ , where  $\tilde{\rho}$  is a smooth mollification of  $\rho$ .

*Proof.* According to Lemma 4.3, we can find  $\mathbf{J} \in C_c^\infty(\Omega, \mathbb{R}^3)$ , with support  $K$ , such that

$$\|\operatorname{div} \mathbf{J} - w\|_{L^2(\Omega)} < \epsilon/2. \quad (50)$$

Now, let  $h \in C_c^\infty(\mathbb{R}^3, [0, 1])$  be a bump function with total integral 1, and  $h_\delta(x) = \delta^{-3}h(x/\delta)$ . Mollify  $\rho$  by convolution with  $h_\delta$ :

$$\tilde{\rho}(x) := (h_\delta * \rho)(x) = \int \rho(x - y) h_\delta(y) dy. \quad (51)$$

Assume  $\delta$  is small enough that  $K + B(0, 2\delta) \subseteq \Omega$ . Then,  $\rho$  is bounded above on  $K + B(0, \delta)$  and  $\rho - \tilde{\rho} \in L^\infty(K)$ .

Define  $\mathbf{u} := \mathbf{J}/\tilde{\rho}$  and compute

$$\operatorname{div}(\rho \mathbf{u}) - \operatorname{div} \mathbf{J} = \operatorname{div} \left( \frac{\rho}{\tilde{\rho}} \mathbf{J} \right) - \operatorname{div} \mathbf{J} = \frac{1}{\tilde{\rho}} (\rho - \tilde{\rho}) \operatorname{div} \mathbf{J} + \frac{1}{\tilde{\rho}} \mathbf{J} \cdot \nabla (\rho - \tilde{\rho}) - \frac{1}{\tilde{\rho}^2} (\rho - \tilde{\rho}) \mathbf{J} \cdot \nabla \tilde{\rho}, \quad (52)$$

keeping in mind that  $\mathbf{J}$  and  $\tilde{\rho}$  are smooth functions, and that the left-hand side of this equation vanishes off  $K$ . Bound the  $L^2(\Omega)$  norms of the three terms in the final expression, as follows:

$$\begin{aligned} \left\| \frac{1}{\tilde{\rho}} (\rho - \tilde{\rho}) \operatorname{div} \mathbf{J} \right\|_{L^2(\Omega)} &\leq \frac{1}{\rho_{\min}} \|\operatorname{div} \mathbf{J}\|_{L^\infty(K)} \|\rho - \tilde{\rho}\|_{L^2(K)}, \\ \left\| \frac{1}{\tilde{\rho}} \mathbf{J} \cdot \nabla (\rho - \tilde{\rho}) \right\|_{L^2(\Omega)} &\leq \frac{1}{\rho_{\min}} \|\mathbf{J}\|_{L^\infty(K)} \|\nabla (\rho - \tilde{\rho})\|_{L^2(K)}, \\ \left\| \frac{1}{\tilde{\rho}^2} (\rho - \tilde{\rho}) \mathbf{J} \cdot \nabla \tilde{\rho} \right\|_{L^2(\Omega)} &\leq \frac{1}{\rho_{\min}^2} \|\mathbf{J}\|_{L^\infty(K)} \|\nabla \tilde{\rho}\|_{L^2(K)} \|\rho - \tilde{\rho}\|_{L^\infty(K)}. \end{aligned} \quad (53)$$

Since  $\rho \in W^{1,2}(\Omega)$ ,  $\lim_{\delta \rightarrow 0} \|\tilde{\rho}\|_{W^{1,2}(K)} = \|\rho\|_{W^{1,2}(K)} < \infty$  and  $\lim_{\delta \rightarrow 0} \|\tilde{\rho} - \rho\|_{W^{1,2}(K)} = 0$ , the right-hand sides in (53) all tend to zero with  $\delta$ . Thus, with  $\delta$  small enough,  $\|\operatorname{div}(\rho \mathbf{u}) - \operatorname{div} \mathbf{J}\|_{L^2(\Omega)} < \epsilon/2$ , hence  $\|\operatorname{div}(\rho \mathbf{u}) - w\|_{L^2(\Omega)} < \epsilon$ .  $\square$

Before proceeding, a few remarks about lower semicontinuity are in order. Saying that an element of  $L^1(\mathbb{R}^n)$  “is” a continuous function is a familiar and benign imprecision, since there is at most one continuous function in the equivalence class of almost everywhere equal functions. Matters are a bit more complicated with lower semicontinuity.

**Definition 4.1.** The *essential lower semicontinuous hull* of a measurable function  $f : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{-\infty, \infty\}$  is defined as

$$\operatorname{lsc} f = x \mapsto \lim_{\delta \downarrow 0} \operatorname{ess\,inf}_{B(x, \delta)} f. \quad (54)$$

In terms of epilevel sets, open set  $\mathcal{O}$  is in  $\{x : \operatorname{lsc} f > c\}$  iff  $f > c$  a.e. on  $\mathcal{O}$ .  $\operatorname{lsc} f$  is the *largest* lower semicontinuous function which is less than or equal to  $f$  a.e. It can always be reduced on a closed set of zero measure while preserving lower semicontinuity and almost everywhere equality. A positive integrable function  $\rho$  has a lower semicontinuous version if and only if  $\int \operatorname{lsc} \rho dx = \int \rho dx$ . For a density  $\rho$ ,  $\operatorname{lsc} \rho$  is the right version to take, because it will not create artificial, extra, connected components of  $\{\rho > 0\}$ .

**Theorem 4.2.** With  $v_{\text{int}} \in \mathcal{V}_{\text{lg}}$ ,  $\mathcal{V}_{\text{lg}}$  has the local HK property.

*Proof.* Let  $\rho = \operatorname{lsc} \rho$  a.e. be a ground-state particle density for both  $v$  and  $v'$  in  $\mathcal{V}_{\text{lg}}$ . Generally, a corresponding (mixed) ground state has a canonical decomposition  $\sum_\alpha c_\alpha |\psi_\alpha\rangle \langle \psi_\alpha|$ , where each  $\psi_\alpha$  is a ground state for both  $v$  and  $v'$ . Assume the theorem holds for densities deriving from vector states; we show that the general case follows. Let  $C$  be a connected component of  $\{\rho > 0\}$  and  $\{C_{\alpha,i}\}_{\alpha,i}$  those of the vector state densities  $\{\operatorname{dens} \psi_\alpha\}$ . (Recall that all these densities are lower semicontinuous.)  $C$  is covered by an *overlapping* collection of  $C_{\alpha,i}$ ’s, on each of which  $v - v'$  must be constant, by the assumption. Thus, the same holds for  $C$ . It therefore suffices to continue under the assumption that  $\rho = \operatorname{dens} \psi$  for a vector state  $\psi$ .

Now, since each connected component  $C$  of  $\{\rho > 0\}$  is a countable union of connected open sets over each of which  $\rho$  is uniformly bounded away from zero, if  $v' - v$  differs from a constant on  $C$ , then it differs from a constant on some bounded connected open set  $\Omega$  over which  $\rho > c > 0$  (strict inequality, note).

Define a cutoff function  $m_R^\ell$  in  $\mathbb{R}^{3\mathcal{N}}$  by

$$m_R^\ell(x) = \prod_{i=1}^{\mathcal{N}} f_R^\ell(|x_i|), \quad f_R^\ell \in C_c^\infty(\mathbb{R}_+; [0, 1]), \quad f_R^\ell(r) = \begin{cases} 1, & r \leq R \\ \text{decreasing to } 0, & R \leq r \leq R + \ell \\ 0, & R + \ell \leq r \end{cases} \quad (55)$$

Using the regions defined by the value of  $m_R^\ell$ , split the particle density as

$$\rho = \int_{m_R^\ell=1} |\psi|^2 d\sigma dx_\perp + \int_{0 < m_R^\ell < 1} |\psi|^2 d\sigma dx_\perp + \int_{m_R^\ell=0} |\psi|^2 d\sigma dx_\perp = \rho_< + \rho_> + \rho_{>>}, \quad (56)$$

where  $\rho_<$ ,  $\rho_>$  and  $\rho_{>>}$  are given by the integrals in the specified order. Since  $\psi$  is continuous and  $\{x : m_R^\ell(x) > 0\}$  has compact closure, both  $\rho_<$  and  $\rho_>$  are continuous for any values of  $R$  and  $\ell$ . Choose  $R$  so that  $\Omega$  is within the  $R$ -ball and  $\rho_< > c$  over  $\Omega$ . Since  $\rho_<$  is increasing to  $\rho$  as  $R \rightarrow \infty$ , Dini's lemma applied to  $\bar{\Omega}$  implies that this can be done.  $\ell$  will be chosen later.

Let  $\epsilon > 0$  be given and apply Lemma 4.4 to get  $\mathbf{J}$  and a mollification  $\tilde{\rho}$  of  $\rho_<$  such that  $\|\operatorname{div}(\rho_< \mathbf{u}) - w\|_{L^2(\Omega)} < \epsilon/2$ , with  $\mathbf{u} = \mathbf{J}/\tilde{\rho}$ .

Modify the lifting of  $\mathbf{u}$  by multiplication with the cutoff function (55):

$$\mathbf{U} := m_R^\ell \cdot \Gamma \mathbf{u}. \quad (57)$$

Now, we have

$$\frac{d\rho}{ds} = \operatorname{div}(\mathbf{u}\rho_<) + \int_{0 < m_R^\ell < 1} \operatorname{div}(\mathbf{U}|\psi|^2) d\sigma dx_\perp \quad (58)$$

The first term on the right-hand side has already been dealt with. Turning to the integral, note that it is a divergence integrated over  $x_2, \dots, x_{\mathcal{N}}$ . Thus, only the first ( $\mathbb{R}^3$ -valued) component of  $\mathbf{U}$  contributes. Secondly, over the range of  $x_1$  values for which  $\mathbf{U} \neq 0$ , the cutoff function  $m_R^\ell$  is independent of  $x_1$ . Keeping that in mind while estimating the two terms of  $\operatorname{div}(\mathbf{U}|\psi|^2) = (\operatorname{div}_1 \mathbf{U}_1)|\psi|^2 + \mathbf{U}_1 \cdot \nabla |\psi|^2$ , we find

$$\left\| \int_{0 < m_R^\ell < 1} \operatorname{div}(\mathbf{U}|\psi|^2) d\sigma dx_\perp \right\|_{L^2(\Omega)} \leq \|\operatorname{div} \mathbf{u}\|_{L^\infty(\Omega)} \|\rho_>\|_{L^2(\Omega)} + \|\mathbf{u}\|_{L^\infty(\Omega)} \|\nabla \rho_>\|_{L^2(\Omega)}. \quad (59)$$

Finally, both terms on the right can be made small by taking  $\ell$  small. Thus, the integral can be made smaller than  $\epsilon/2$  in  $L^2$  norm, with the result that  $\|w - d\rho/ds\|_{L^2(\Omega)} < \epsilon$ .  $\square$

It follows immediately from this theorem that if  $\rho$  satisfies the further hypothesis of not vanishing anywhere, the strongest possible conclusion about potential uniqueness follows.

**Corollary 4.1.** *With  $v_{\text{int}} \in \mathcal{V}_{\text{lg}}$ , if  $\operatorname{lsc} \rho$  is everywhere nonzero and equals  $\rho$  a.e., then  $\Delta \mathcal{V}_{\text{lg}}(v_{\text{int}}, \rho)$  contains only constants. [If  $\operatorname{lsc} \rho$  is inequivalent to  $\rho$ , then  $\mathcal{V}_{\text{lg}}(v_{\text{int}}, \rho) = \emptyset$ .]*

Now we turn our attention to the smaller classes of potentials.

**Theorem 4.3.** *With  $v_{\text{int}} \in \mathcal{V}_{\text{md}}$ ,  $\mathcal{V}_{\text{md}}$  has the weak HK property.*

*Proof.* An argument very similar to that used in the proof of Thm. 4.2 reduces the mixed state case to that of vector states. Thus, we assume  $\rho$  is a ground state particle density for both  $v$  and  $v'$  in  $\mathcal{V}_{\text{md}}$ , with a corresponding vector ground state  $\psi$ . For convenience, we assume that the ground state energies are both zero; this can be arranged by adding constants to  $v$  and  $v'$ .

Let  $\mathcal{C}$  denote the set of connected components of  $\{\rho > 0\}$ , and consider the situation in  $U^{\mathcal{N}}$  (in  $\mathcal{N}$ -particle configuration space  $\mathbb{R}^{3\mathcal{N}}$ ) for an arbitrary  $U \in \mathcal{C}$ . As in the argument of the Introduction,  $[\Gamma(v' - v)]\psi = 0$ . But, Thm. 4.2 shows that  $v' - v$  is a constant throughout  $U^{\mathcal{N}}$ . Therefore, either  $v' = v$  on  $U$  or  $\psi$  vanishes a.e. on  $U^{\mathcal{N}}$ . Since both  $v$  and  $v_{\text{int}}$  are in  $\mathcal{V}_{\text{md}}$ , the weak UCP Thm. 3.2 of Schechter & Simon is applicable. Therefore, vanishing of  $\psi$  over  $U^{\mathcal{N}}$  implies that it vanishes off the union of the exceptional sets of  $v$  and  $v'$ . Since the latter have zero measure, that would imply that  $\psi \equiv 0$ . The contradiction establishes that  $v = v'$  over every element of  $\mathcal{C}$ .  $\square$

By restricting  $v_{\text{int}}$  further, it will be possible to attribute vanishing of  $\rho$  on a set of nonzero measure to the ‘‘singularities’’ of the external potential.

**Corollary 4.2.** *With  $v_{\text{int}} \in \mathcal{V}_{\text{sm}}$ , suppose  $v \in \mathcal{V}_{\text{md}}$  has a ground-density  $\rho$ . If  $v$  is essentially bounded on an open set  $U$ , then  $U \cap \{\rho = 0\}$  has zero measure.*

*Proof.* Assume  $v$  is essentially bounded over  $U$ . Then both the external potential and the interaction potential are bounded over  $U^{\mathcal{N}}$ . But, if  $A := U \cap \{\rho = 0\}$  has nonzero measure, then  $\psi$  vanishes on the nonzero-measure set  $A^{\mathcal{N}} \subset U^{\mathcal{N}}$ . This implies, by Prop. 3.1 or by the result of de Figueiredo & Gossez, that  $\psi$  has a zero of infinite order. According to the applicable strong UCP (Jerison & Kenig or Müller),  $\psi$  vanishes over  $U^{\mathcal{N}}$ . But, from the proof of Thm. 4.3, we know that to be impossible.  $\square$

Another way to put the conclusion of this theorem, closer to the phrasing in the Introduction, is to say that any version of  $\{|v| \geq c\}$  is dense in  $\{\rho\}$  almost everywhere for every  $c > 0$ . The words “any version” refer to the fact that  $\{|v| \geq c\}$  is defined only up to a set of measure zero (but such a difference set could be dense in  $\mathbb{R}^3$ ).

The natural completion of our set of theorems is

**Theorem 4.4.** *With  $v_{\text{int}} \in \mathcal{V}_{\text{sm}}$ ,  $\mathcal{V}_{\text{sm}}$  has the strong HK property.*

This follows immediately from the Jerison & Kenig (or even Müller) strong UCP, combined with the reduction of de Figueiredo & Gossez. It is stronger than Thm. 4.1, but also requires more machinery.

## 5. DISCUSSION: WHAT IS THE POINT OF THE HOHENBERG-KOHN THEOREM?

The time has come to assess our results and attempt to put them in context. That, in turn, requires an inquiry into the rôle of the Hohenberg-Kohn theorem in DFT. Let us briefly try some attitudes.

Hohenberg and Kohn<sup>1</sup> wrote “Thus  $v(\mathbf{r})$  is (to within a constant) a unique functional of  $n(\mathbf{r})$ ; since, in turn,  $v(\mathbf{r})$  fixes  $H$  we see that the full many-particle ground state is a unique functional of  $n(\mathbf{r})$ .” Using said ground-state  $\psi$  with  $\text{dens } \psi = \rho$ , they go on to define the intrinsic energy as  $F[\rho] = \langle \psi | H_0 | \psi \rangle$ . Can we say that the first Hohenberg-Kohn theorem has a part in holding this definition down, now rendering obsolete since the modern definition of  $F$  uses the constrained-search method? No. For, while existence of *at least one* ground state with density  $\rho$  (the infamous “ $V$ -representability” problem) is required here, it is completely irrelevant whether either the ground-state or the potential is unique.

Recall the quotation from Martin in the introduction. Similar statements, are not uncommon in the literature. For example, Kohn<sup>35</sup> says, in his Nobel lecture, “Hence  $n(r)$  determines implicitly all properties derivable from  $H$  ... such as: the many-body eigenstates ... , the two-particle Green’s function ... , the frequency dependent electric polarizability, and so on. We repeat that all this information is implicit in  $n(r)$ .” What is this about? Inverse problems are of importance in physics, but problems to which DFT is applied seem not to be of that variety. The external potential is *known*. (In the sense relevant here. Of course, investigation may be needed to find total-energy-minimizing nuclear positions, for example.) There is no actual calculational proposal here. It seems, instead, to amount to the claim that no “information” is lost on passing from ground states to ground state densities (clearly there cannot be a gain). Now, a simple argument given in the introduction shows that, for any class  $\mathcal{V}$  of potentials,  $\Delta\mathcal{V}(v_{\text{int}}, \rho)$  contains only constants for all  $\rho$  if and only if the same is true of  $\mathcal{V}(v_{\text{int}}, \psi)$  for all  $\psi \in \mathcal{H}_{\mathcal{N}}$  ( $\mathcal{V}(v_{\text{int}}, \psi)$  being an obvious extension of the notation). If  $\mathcal{V}$  has the strong HK property with respect to  $v_{\text{int}}$ , should that be considered enough for “no loss”? Perhaps. But it may be that this is just a reflection of the poverty of  $\mathcal{V}$ . The subclasses of  $\mathcal{V}_{\text{af}}$  considered in Thm. 4.1 can be accused of exactly that. For a class of potentials lacking the strong HK property, a more fine-grained analysis is necessary. In such a case, there is an evident *sufficient* condition for  $\Delta\mathcal{V}(v_{\text{int}}, \psi)$  to contain only constants, namely,  $\psi$  is almost everywhere nonzero. Thm. 4.2 shows that for  $v_{\text{int}} \in \mathcal{V}_{\text{lg}}$ ,  $\Delta\mathcal{V}_{\text{lg}}(v_{\text{int}}, \rho)$  contains only constants if  $\rho$  is almost everywhere nonzero. Arguably, such a result could be considered more impressive. After all, a density can be nonvanishing almost everywhere without the corresponding wavefunction having that property. This suggests that an emphasis on “no information loss” is misplaced, the point being rather to jettison irrelevant information. If so, then our results might be held to be stronger evidence for the value of working with particle density than the naïve Hohenberg-Kohn theorem would be.

Another attitude argues that realistically we should only be concerned with “physical” potentials. Which are those? Shall we say that, since the DFT under discussion is a nonrelativistic approximation and point-like nuclei are part of that approximation, that  $\mathcal{V}_{\text{mol}}$  is indicated, and Thm. 4.1 is all we need? Or that nuclei are actually extended, so that the potentials are bounded and continuous? The two positions are, of course, incompatible; both trade on a too-narrow notion of “physical”. The first, at least, is incompatible with the actual practice of DFT. Modern methods of manipulating cold atomic gases allow highly tailorable external and interaction potentials, and there is no reason DFT methodology cannot be applied to them<sup>36,37</sup>. Trap potentials, idealized as positive and unbounded at infinity, at least should be considered. That was part of the motivation for our loose constraints on  $v^+$ . DFT calculations in the Kohn-Sham form routinely employ “non-physical” with non-interacting electrons.



With the failure of transparently physical considerations to definitively answer the titular question of this section, or unambiguously indicate an appropriate scope, it probably makes sense to fall back to a softer position. Arguably, the central object of DFT is the intrinsic energy functional  $F$ , or relatedly, if not quite equivalently, the exchange-correlation energy. From such a position, we see the various results about HK properties as providing complementary information about the “derivative” (really, subdifferential) of the intrinsic energy. But the results should not be isolated from the way they were obtained. The methods used, which keep the density squarely in view, demonstrate the power of thinking in terms of density.

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